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14. ABSTRACT The present program aimed to study the dynamics of droplet collision and flame-flow interaction that are of relevance to liquid-fueled turbulent combustion in propulsive devices. Four classes of phenomena were specifically investigated, namely: (1) The dynamics of binary droplet collision, especially on the criterion for the breaking of the inter-droplet surfaces which enables droplet merging. (2) The dynamics of droplet-droplet collision of dissimilar liquids, showing that the initiation of droplet internal superheating and hence microexplosion can be greatly facilitated by the presence of air bubbles entrained upon coalescence of the colliding droplets. (3) The dynamics of droplet-film collision, especially on the influence of the film thickness in effecting droplet bouncing versus absorption. (4) The dynamics of flame motion when it is subjected to the combined hydrodynamic and body-force instabilities and freestream vortical motion.						
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Final Technical Report
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**DYNAMICS OF DROPLET COLLISION AND
FLAMEFRONT MOTION**
(AFOSR F49620-03-1-0136)

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BACKGROUND

This research program aimed to investigate two major categories of phenomena that take place in propulsion devices, namely the dynamics of droplets and of flames. In terms of droplet dynamics, it is noted that one of the rate-limiting processes in liquid-fueled propulsive devices is the time needed to vaporize the liquid fuel (or oxidizer) so that gas-phase mixing, heating and consequently reaction can take place. In order to achieve rapid gasification, it is necessary to first finely atomize the liquid fuel such that the total surface area of the droplet ensemble is maximized for heat and mass transfer. Fine atomization, however, is not sufficient to ensure that the initial spray characteristics are optimized, for two reasons. The first factor for consideration is that, in the dense spray region immediately downstream of the spray injector, the droplets can collide and, depending on the outcome of such a collision, modify the initial spray statistics. Such collisions will certainly occur in the impinging-jet type of atomizers in which the dominant motion of the two groups of droplets is directed towards each other. For conventional injectors, the randomness of the droplet and gas motion is also expected to cause frequent droplet collision. Our study has identified a rich variety of outcomes upon the collision of two droplets. For example, they can either merge to form a larger droplet, or bounce away from each other. Furthermore, the collision event has been found to be inelastic due to the viscous loss associated with the motion within the liquid, leading to dissipation of the kinetic energy of the droplets and hence a net reduction of the spray inertia. All these will alter the initial condition of the spray and the subsequent spray development and burning responses. The second factor for consideration is that, depending on the spray pattern and the proximity of the spray to the surfaces of the combustor, some droplets could also impinge onto these surfaces, resulting in either bouncing off or wetting of the surface. The subsequent gasification rate of the liquid mass would obviously depend on whether it takes place at the droplet or the combustor surface. Ultimately, the burner performance in terms of its thrust and combustion stability will be accordingly affected through the outcomes of these droplet-droplet and droplet-wall collisions. The need to accurately control and understand the initial spray characteristics can hardly be over-emphasized.

During the reporting period we have systematically quantified and understood droplet-droplet and droplet-surface collisions. The investigation has involved both experimentation and computational simulation. Substantial progress has been made in various aspects of these complex phenomena, as will be discussed in the following. It is to be emphasized that our studies on droplet collision have now progressed to the most

exciting stage of attaining qualitative understanding and quantitative predictability, namely the ability to describe the destruction and thereby merging of the colliding interfaces. The knowledge gained will have significant impact on the general discipline of interfacial science.

In parallel with the studies on droplet collision, we have also conducted extensive computational simulations of the dynamics of flame surfaces. This endeavor was initiated upon the recognition that the computational algorithm developed for droplet collision can be readily modified for the study of flame motion in complex flow fields. Specifically, both problems involve the tracking of deformable interfaces separating two media of vastly different densities: the interface is the liquid surface in droplet collision and the flame surface in flame dynamics. The need to accurately track the flame surface in simulating the complex flow field in combustors is quite apparent. That is, for many practical situations the chemical reaction time is much faster than the flow time, implying that the flame can be approximated by infinitesimally-thin surfaces over which reactants are consumed and heat is generated. These surfaces possess their own propagation velocities while at the same time are convected by the prevailing flow. The overall heat release rate of the combustion process then directly depends on the surface area and propagation velocity of the flame.

We shall now present high-lights of our research accomplishments for the sponsored program.

1. Droplet-Droplet Collision

Our previous studies on droplet-droplet collision showed that, depending on the collision Weber number, We , the collision event can result in either merging or bouncing of the droplets. Phenomenologically, the propensity for bouncing or merging depends on the readiness with which the gaseous mass in the inter-droplet gap can be squeezed out by the colliding interfaces such that they can make contact at the molecular level, leading to their destruction and thereby resulting in merging.

The lack of a clear criterion on the instant of surface rupture has caused considerable uncertainty in the computational simulation of the collision event and consequently understanding of the collision and merging dynamics. Specifically, since the development of the shape and phase of droplet deformation is driven through the

interplay between the surface condition and the flow field, comparison between the global experimental and calculated collision images would allow the extraction of the detailed flow structure such as the contour and dynamics of the droplet surface and the distributions of pressure, velocity, and energy budget. This information cannot be readily acquired experimentally due to the small dimension of the phenomena of interest, especially those within the inter-droplet gap. Furthermore, because of the richness of the phenomena involved, and because of the challenging need to track the displacement of a deformable, sharp interface, computational simulation of the experimental collision images can also serve to validate hydro-codes. However, since these hydro-codes are usually based on continuum mechanics, while the final stage of the interfacial dynamics leading to merging must necessarily involve rarified flows within the narrow interfacial gap as well as molecular forces, the lack of such basic information renders it fundamentally impossible to simulate the interface rupture from first principles. This difficulty was circumvented by artificially, and quite arbitrarily, removing the interfaces at a certain instant when they are sufficiently close to each other. The fidelity of the simulation then sensitively depends on the instant at which the rupture is implemented.

In the present study we have observed that the occurrence and the instant of merging can be identified through a distinct change in the cuspy contour of the imaged interface, as shown in the 4th and 5th experimental images of Fig. 1. By further recognizing that such an instant can be time resolved with sufficient accuracy such that, by using it as an input to the computational simulation based on continuum mechanics, the evolution of the experimental collision images subsequent to merging can be satisfactorily simulated. Figure 1 shows the close agreement between the experimental and simulated images.

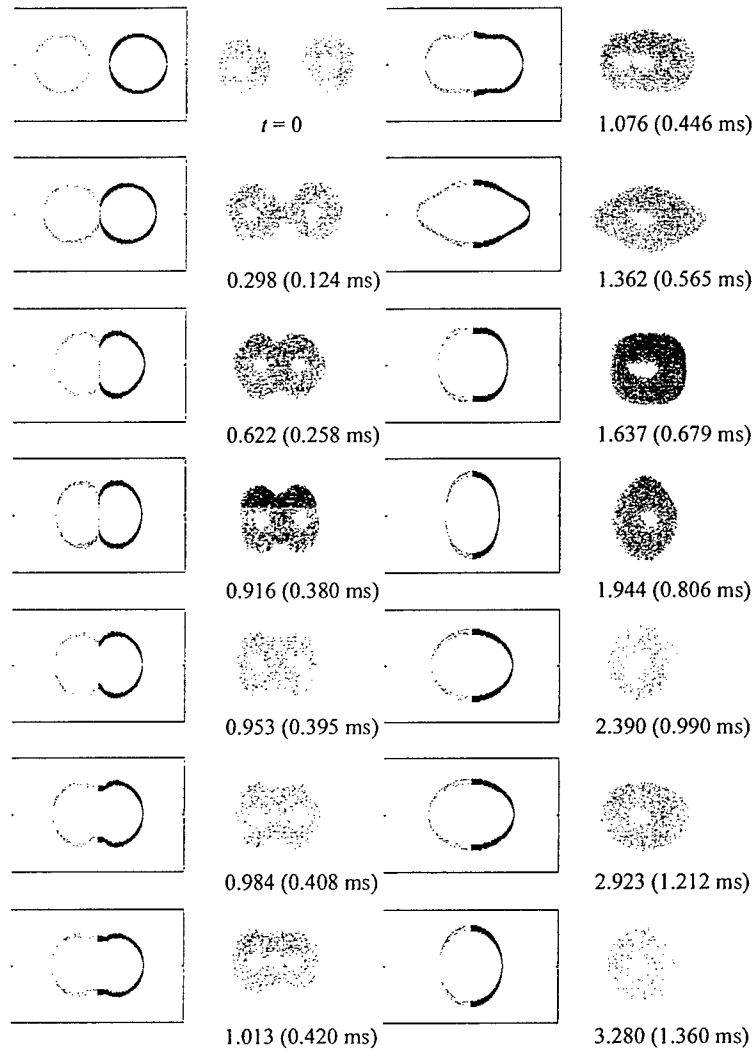


Figure 1

To further demonstrate the sensitivity of the collision dynamics to the specification of this merging instant, Fig. 2 shows the simulated images when the assumed instant of surface rupture was either advanced or delayed. It is seen that qualitatively different outcomes are predicted.

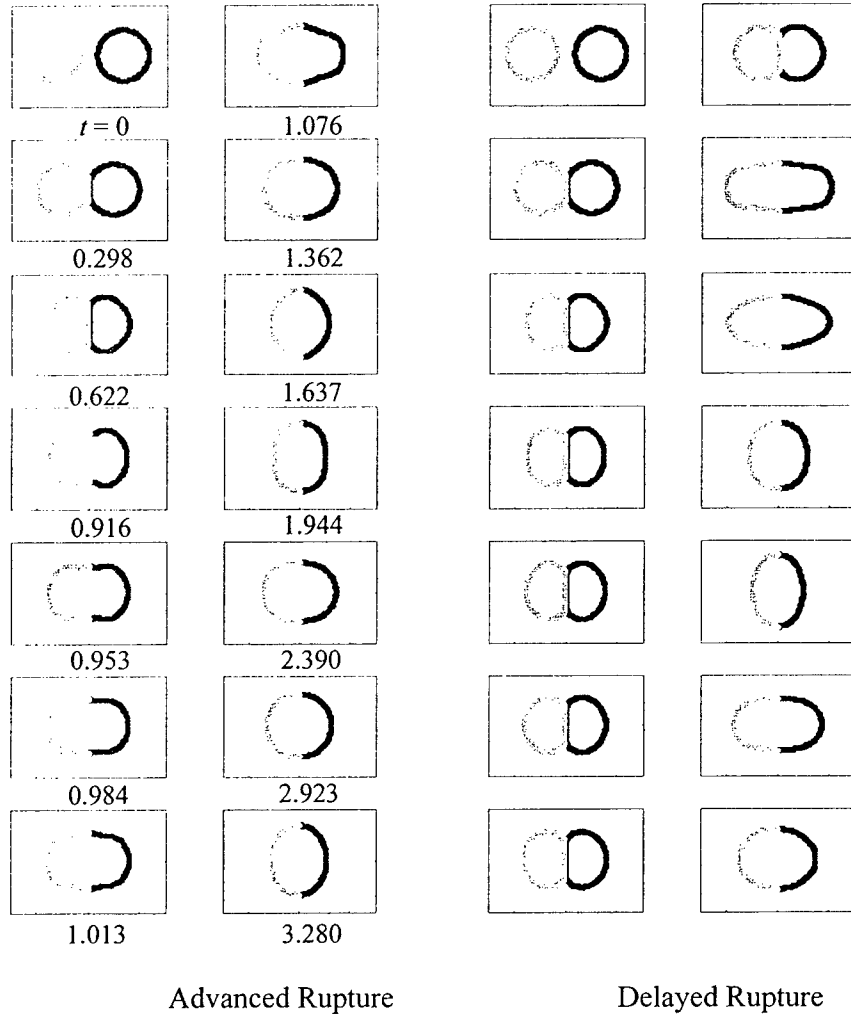


Figure 2

Having established the adequacy of this empirically enabled computational simulation approach, we further studied the various issues related to the merging and bouncing aspects of the collision dynamics, including the energy budget, the flow field characteristics, and evolution of the geometry and dynamics of the inter-droplet gap, with emphasis on the transition between bouncing and merging regimes. In particular, recognizing the essential importance of the van der Waals force in effecting the final merging of the surfaces, we have added such a force in the governing equations. Since merging is expected to occur at the rim of the interface (see Fig. 3), Fig. 4 shows the evolution of the location of the rim of the impinging droplet interface. It is seen that at a certain instant it indeed precipitously decreases to zero, indicating the attainment of

merging. However, it was also found that in order to achieve merging at the observed instant of surface rupture, the Hamaker constant (A^*) of the van der Waals force needs to be artificially increased by three to six orders of magnitude. This is to be expected because the computational code was based on continuum mechanics, while the flow in the interfacial gap during the final stage of merging is clearly that of rarefied flow. Thus the computed pressure within the gap is higher, implying that an artificially augmented van der Waals force is needed to effect merging.

This work is reported in Publication No. 1.

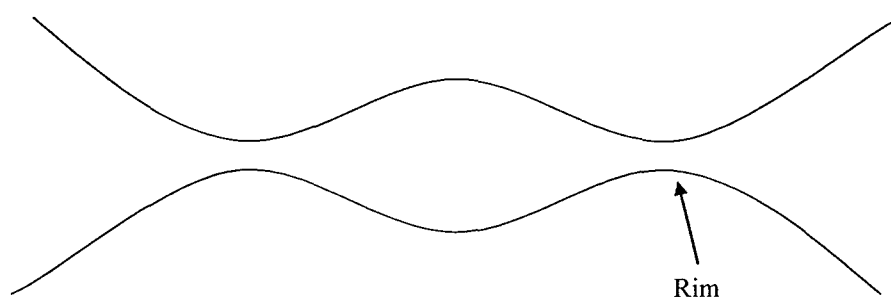


Figure 3

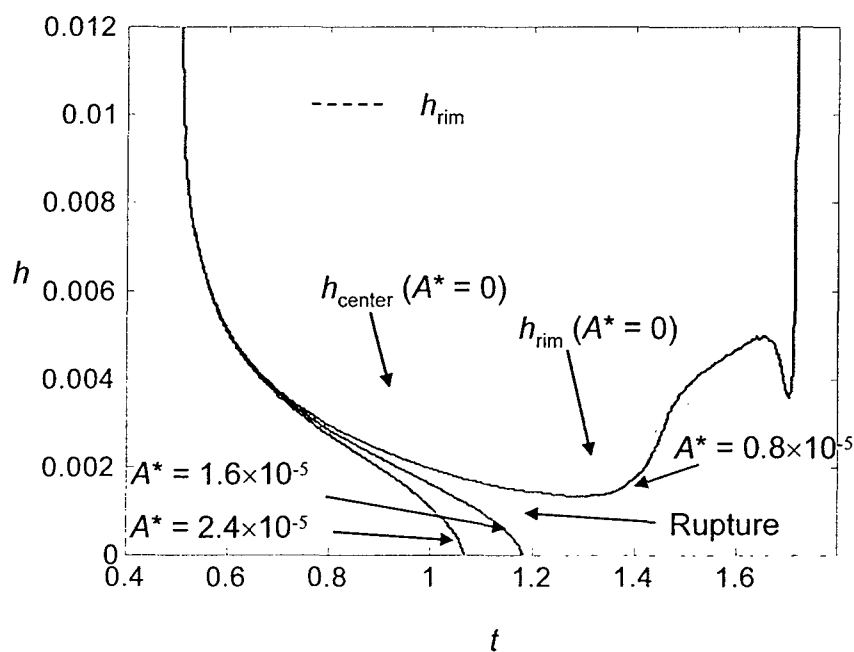


Figure 4

2. Bubble Entrapment and Droplet Micro-explosion

Referring back to Fig. 3, it is reasonable to anticipate that, if coalescence indeed occurs at the rim, then a gas bubble will be entrapped within the coalesced mass. Consequently, when the coalesced droplet undergoes combustion, the embedded bubble will expand as the droplet is heated up. This can eventually burst the droplet.

The phenomenon of droplet micro-explosion has been known since the 1970s. Specifically, it was observed that droplets of certain fuels or fuel blends tend to explode catastrophically at a certain instant during burning. The mechanism responsible for such an occurrence is the superheating of the liquid elements within the droplet interior, induced either by the presence of some volatile components, or by the heat generated through the decomposition of a monopropellant within the droplet interior. The present mechanism, namely the heating and hence expansion of the entrapped gas bubbles upon droplet merging, is therefore distinctively different than those identified previously.

Figure 5 shows the presence of a gas bubble in a merged droplet. Figure 6 shows the flame streaks of two streams of downwardly falling droplets, with the right one generated by the collision between two droplets, while the left one generated as a single stream. It is seen that only the right streak, representing the situation with embedded air bubbles, exhibits micro-explosion.

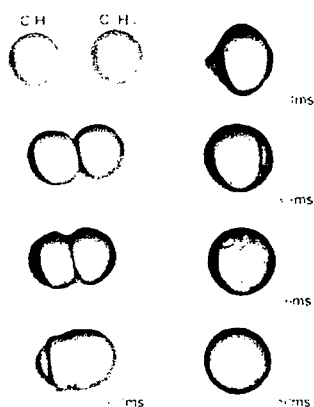


Figure 5

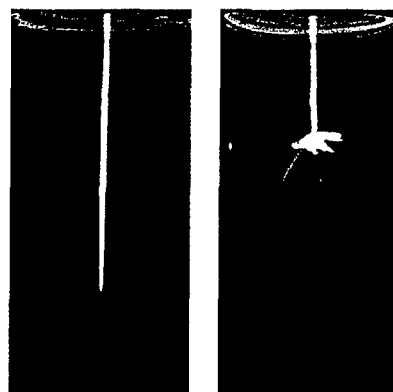


Figure 6

The possible existence of droplet micro-explosion holds significant potential for enhanced atomization. That is, since there is a limit on the extent of atomization achievable through spraying, the occurrence of micro-explosion can be considered to be a secondary atomization process through which finer droplets can be produced. Furthermore, it more than compensates for the negative aspect of droplet coalescence in

that it will eventually cause the production of secondary droplets whose sizes are smaller than those of the original colliding droplets.

This work is reported in Publication Nos. 2, 3, and 4.

3. Droplet-Surface Collision

Extending our knowledge on droplet-droplet collision, it is reasonable to expect that the outcome of droplet-surface collision must fundamentally depend on two factors, namely whether the surface is dry or wet, and the thickness of the film when it is wet. Experimental results obtained for the wet surface show that the collision outcome depends sensitively on two parameters, namely the film thickness relative to the droplet radius, and the impact inertia characterized by the droplet Weber number. Figure 7 shows the regime diagram of the collision outcomes, with the ordinate being the film thickness scaled by the droplet radius (H). It is seen that bouncing and coalescence are respectively favored for small and large We , which is reasonable. Furthermore, there are three additional observations that are particularly noteworthy. First, there is a range in We within which increasing the film thickness leads the outcome to change from coalescence to bouncing, to coalescence again, and to bouncing again. Second, as the film becomes very thin, of the order of a few microns, coalescence always occurs. Third, the boundary of $We \sim 14.3$ beyond which coalescence always occurs is the same value observed for droplet-droplet collision.

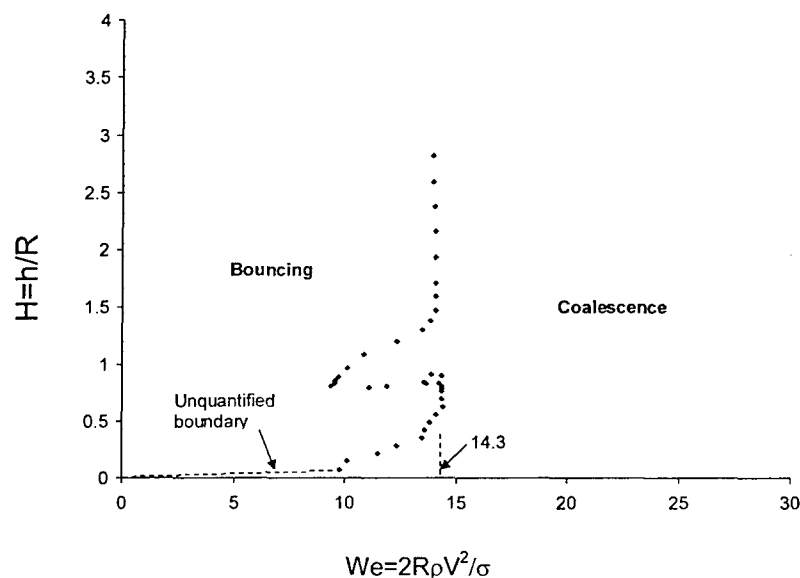


Figure 7

Figures 8 and 9 respectively show the time-resolved collision events of a bouncing and a coalescence outcome.

Detailed simulation of the collision event shows that absorption of the droplet by the film for thin and thick films respectively occur at the rim and the center of the droplet interface, indicating the importance of the solid surface in constraining the impacting droplet and hence promoting merging.

This work is reported in Publication No. 5. We are also pleased to note that this paper was selected as the best paper presented at the conference.

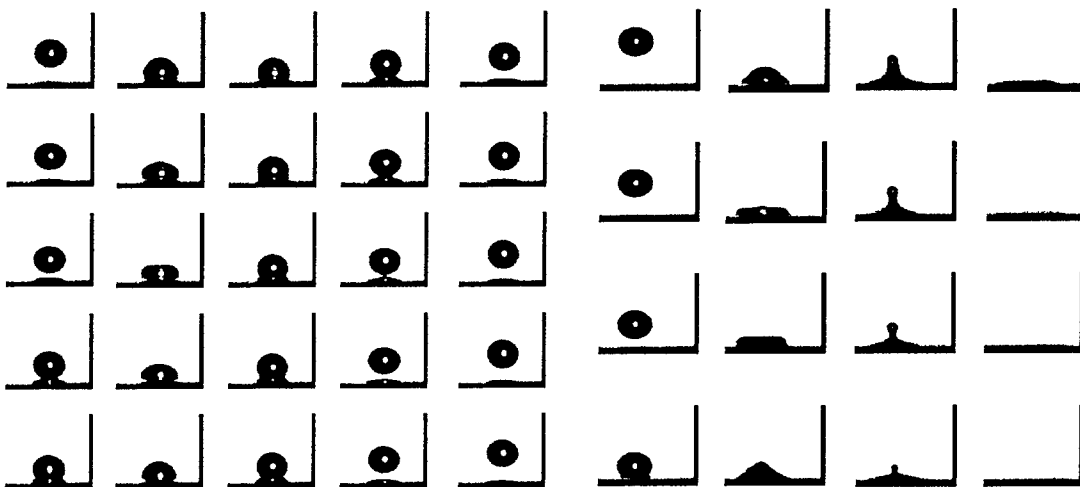


Figure 8

Figure 9

4. Flame Propagation with Hydrodynamic and Body-Force Instabilities in Vortical Flows

Extending our previous studies on the role of hydrodynamic (Darrieus-Landau) instability in the wrinkling of flame surface at the incipient stage, we have further investigated the flame dynamics in the course of long-time evolution when interactions between the flame front, the instability, and the vortical flow result in highly convoluted flame configurations. It is shown that, with the inherent mechanisms of merging and division of flame cells at multiple scales that are generated by the hydrodynamic instability, propagation of flame wrinkles can evolve to a quasi-stable state characterized by either a solitary wave or chaotic motion associated with the corrugated front. If the vortical flow is sufficiently strong, however, the flame geometry is contorted by the vortices while the effect of hydrodynamic instability diminishes. Therefore, according to the relative

magnitudes of the intensity of the hydrodynamic instability, determined by the density ratio as well as the curvature parameter that is related to the flame thickness, and the strength of the vortices, the interaction pattern can be classified as flame-instability dominated, flow dominated, and a hybrid of the two. We further studied the effect of gravity on the reacting flow. It is found that, while wrinkled flames can be stabilized by sufficiently strong, negative gravity associated with downward flame propagation, wrinkles with short wavelengths remain intact while those with long wavelengths are suppressed. As such, compared to the zero-gravity condition, the reduced multiplicity of cellular scales and the subsequent decreasing interactions between multi-scale wrinkles diminish the chaotic motion. On the other hand, when positive gravity is introduced, the unsteady evolution characterized by incessant merging and division of cells is suppressed. This is in contrast to previous realization in that, while a flame is readily distorted to a large wrinkle at the incipient stage of Darrieus-Landau instability, subsequent stability due to the coupling of Darrieus-Landau and Rayleigh-Taylor instabilities prevents excitation of secondary Darrieus-Landau instability and consequently renders the entire structure more stable. However, if the positive gravity is sufficiently large, the ordered pattern degenerates and highly irregular geometry of the flame surface is formed without specific cell structure. This is the typical manifestation of Rayleigh-Taylor instability caused by buoyant force exerted on an interface with density jump.

Archival Publications

The following papers report work sponsored by the present program.

1. "On the dynamics of head-on droplet collision: experiment and simulation," by K. L. Pan and C. K. Law, Paper No. AIAA 2004-1159, 42nd Aerospace Sciences Meeting, Reno, NV, Jan. 5-8, 2004. Submitted for publication in *Journal of Fluid Mechanics*.
2. "On the burning and microexplosion of collision-generated bi-component droplets: miscible fuels," by C. H. Wang, W. G. Hung, S. Y. Fu, W. C. Huang, and C. K. Law, *Combustion and Flame*, Vol. 134, pp. 289-300 (2003).

3. "On the burning characteristics of collision-generated water/hexadecane droplets," C. H. Wang, W. G. Hung, S. Y. Fu, W. C. Huang, and C. K. Law, *Combustion Science and Technology*, Vol. 176, No. 1, pp. 71-93 (2004).
4. "Combustion and microexplosion of collision-merged methanol/alkane droplets," by C. H. Wang, S. Y. Fu, L. J. Kung, and C. K. Law, *Proceedings of the Combustion Institute*, Vol. 30, pp. 1965-1972 (2005).
5. "Dynamics of droplet-film collision," by K.L. Pan and C.K. Law, Paper No. AIAA 2005-0352, 43rd Aerospace Sciences Meeting, Reno, NV, Jan. 10-13, 2005.

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